REPORT DOCUMENTATION PAGE	Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
02-02-2011	Final Report	1-May-2004 - 31-Oct-2010

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Development of systematic approaches for calibration of subsurface transport models using hard and soft data on system characteristics and behavior	W911NF-04-1-0169
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER 611102
6. AUTHORS Tissa H. Illangasekare, Toshihiro Sakaki	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES	8. PERFORMING ORGANIZATION REPORT NUMBER
Colorado School of Mines Colorado School of Mines 1500 Illinois Street Golden, CO 80401 -	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSOR/MONITOR'S ACRONYM(S) ARO
	11. SPONSOR/MONITOR'S REPORT NUMBER(S) 45814-EV.1

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES

The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

This research seeks to extend and combine tools for parameter estimation and geostatistical simulation for use with groundwater flow and transport models used by the Army. Funds were added to include a research task to investigate the soil moisture distribution in the shallow subsurface affected by buried objects and heterogeneity in the soil under various surface conditions. The primary aims of the project are to: (1) develop an improved understanding of how to include in a systematic way the geostatistical description of aquifer heterogeneity to

15. SUBJECT TERMS

model calibration, data assimilation, subsurface transport

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Tissa Illangasekare
UU	UU	UU	UU		19b. TELEPHONE NUMBER 303-384-2126

Report Title

Development of systematic approaches for calibration of subsurface transport models using hard and soft data on system characteristics and behavior

ABSTRACT

This research seeks to extend and combine tools for parameter estimation and geostatistical simulation for use with groundwater flow and transport models used by the Army. Funds were added to include a research task to investigate the soil moisture distribution in the shallow subsurface affected by buried objects and heterogeneity in the soil under various surface conditions. The primary aims of the project are to: (1) develop an improved understanding of how to include in a systematic way the geostatistical description of aquifer heterogeneity to calibration, (2) develop methods to condition parameter estimation to results from pumping tests/tracer tests and lithology data, (3) use sparsely sampled lithology and drawdown data to determine calibration parameters at the field scale, (4) develop a data set that describes the spatial and temporal behavior of soil moisture retention in simple heterogeneous systems and understand the behaviors at a resolution that is significantly finer (order of ~cm) than those used in other applications, (5) Develop a fundamental scientific basis for understanding heat, liquid water and water vapor transport around buried objects in the shallow subsurface and (5) develop a better understanding of the characteristics of disturbed soils through the characterization of hydraulic/thermal properties.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

1. Sakaki, T., A. Limsuwat, and T. H. Illangasekare (2011, in press), An improved air pressure measuring method and demonstrated application to drainage in heterogeneous soils, Vadose Zone Journal, V10-0121.
2. Smits, K. M., A. Cihan, T. Sakaki, and T. H. Illangasekare (2011, in press), Evaporation from soils under thermal boundary conditions: Experimental and modeling investigation to compare equilibrium and non-equilibrium based approaches, Water Resour. Res., 2010WR009533. (PDF attached)
3. Sakaki, T., A. Limsuwat, and T. H. Illangasekare (2011, in press), A simple method for calibrating dielectric soil moisture sensors: Laboratory validation in sands, Vadose Zone Journal, V10-0036.
4. Sakaki, T., D. M. O'Carroll, and T. H. Illangasekare (2010), Direct quantification of dynamic effects in capillary pressure for drainage and wetting cycles, Vadose Zone Journal, 9:424-437, DOI: 10.2136/vzj2009.0105. (PDF attached)
5. Smits, K. M., T. Sakaki, A. Limsuwat, and T. H. Illangasekare (2010), Thermal conductivity of sands under varying moisture and porosity in drainage–wetting cycles, Vadose Zone Journal, 9:172-180, DOI: 10.2136/vzj2009.0095. (PDF attached)
6. Sakaki, T., C. C. Frippiat, M. Komatsu, and T. H. Illangasekare (2009), On the value of lithofacies data for improving groundwater flow model accuracy in a three-dimensional laboratory-scale synthetic aquifer, Water Resour. Res., 45, W11404, doi:10.1029/2008WR007229. (PDF attached)
7. Sakaki, T., A. Limsuwat, K. M. Smits, and T. H. Illangasekare (2008), Empirical two-point ?-mixing model for calibrating the ECH2O EC-5 soil moisture sensor in sands, Water Resour. Res. Special Collection on Hydrologic Measurement Methods, 44, W00D08, doi:10.1029/2008WR006870 (4th place most downloaded article for two weeks). (PDF attached)
8. Sakaki, T., and T. H. Illangasekare (2007), Comparison of height-averaged and point-measured capillary pressure - saturation relations for sands using a modified Tempe cell, Water Resour. Res., 43, W12502, doi:10.1029/2006WR005814. (PDF attached)

Number of Papers published in peer-reviewed journals: 8.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 0.00

(c) Presentations

1. Smits, K. M., A. Cihan, T. Sakaki, S. Howington, J. Peters and T. H. Illangasekare, (Abstract submitted), The effect of heterogeneity on evaporation/condensation in soil – numerical simulation, MODFLOW and More 2011: Integrated Hydrologic Modeling, June 6-8, 2011, Colorado School of Mines, Golden, Colorado.
2. Sakaki, T., A. Limsuwat, and T. H. Illangasekare (2010), Water flow and retention in coarse soil pockets in the shallow subsurface, AGU Fall meeting, December 13-17, San Francisco, CA.
3. Smits, K. M., A. Cihan, T. Sakaki and T. H. Illangasekare (2010), Evaporation from soils under thermal boundary conditions: Experimental and modeling investigation to compare equilibrium and non-equilibrium based approaches, AGU Fall meeting, December 13-17, San Francisco, CA.
4. Smits, K. M., A. Cihan, T. Sakaki, and T. H. Illangasekare (2010), Evaporation from soils under thermal boundary conditions: Experimental and modeling investigation to compare equilibrium and non-equilibrium based approaches, The proceedings of the 27th Army Science Conference, November 29-December 2, 2010, Orlando, Florida.
5. Cihan, A., T. H. Illangasekare, A. Limsuwat, and T. Sakaki (2010), Upscaling soil hydraulic functions based on connectivity in heterogeneous porous media, Proceedings of the 30th Annual American Geophysical Union Hydrology Days, March 22-24, 2010, ed. J. A. Ramirez, Colorado State University, Fort Collins, CO.
6. Smits, K. M., Cihan, A., T. Sakaki, and T. H. Illangasekare (2010), Shallow subsurface soil moisture behavior as affected by heat source boundary conditions: Experimental and modeling investigation, Proceedings of the 30th Annual American Geophysical Union Hydrology Days, March 22-24, 2010, ed. J. A. Ramirez, Colorado State University, Fort Collins, CO.
7. Limsuwat, A., T. Sakaki, and T. H. Illangasekare (2010), Experimental study on role of air flow in transient water retention behavior in one dimensional layered system subjected to drainage and wetting, Proceedings of the 30th Annual American Geophysical Union Hydrology Days, March 22-24, 2010, ed. J. A. Ramirez, Colorado State University, Fort Collins, CO.
8. Sakaki, T., C. C. Frippiat, M. Komatsu, and T. H. Illangasekare (2010, Invited), How many boreholes are needed to estimate hydrofacies structure in the subsurface with reasonable accuracy?, Proceedings of the "International Symposium on Environmental Science and Technology", 133-138, February 22-23, 2010, Okayama University, Okayama, Japan.
9. Sakaki, T., A. Limsuwat, and T. H. Illangasekare (2009), Role of air on local water retention behavior in the shallow heterogeneous vadose zone, AGU Fall meeting, Poster No. H31A-0749, December 14-18, San Francisco, CA.
10. Smits, K. M., A. Cihan, T. Sakaki, and T. H. Illangasekare (2009), Heat-induced evaporation in the shallow subsurface: Experimental and modeling investigation, AGU Fall meeting, Poster No. H31A-0747, December 14-18, San Francisco, CA.
11. Komatsu, M., C. C. Frippiat, T. Sakaki, and T. H. Illangasekare (2009), A simple Bayesian method to combine lithofacies data with drawdown measurements when calibrating a groundwater flow model, AGU Fall meeting, Poster No. H43F-1088, December 14-18, San Francisco, CA.
12. Illangasekare, T. H., T. Sakaki, B. Petri, and A. Limsuwat (2009), Vapor intrusion from entrapped NAPL sources and groundwater plumes: Process understanding and improved modeling tools for pathway assessment, The SERDP/ESTCP Partners Symposium, December 1-3, 2009, Washington DC.
13. Illangasekare, T. H., T. Sakaki, K. M. Smits, A. Limsuwat, and J. M. Terrés-Nícoli (2009, Invited), Understanding Soil Moisture Processes for the Modeling of Near Surface Unsaturated Zone: Experimental Investigations in Multi-scale Test Systems, ModelCARE 2009, The 7th International Conference on Calibration and Reliability in Groundwater Modeling "Managing Groundwater and the Environment", September 20-23, Wuhan, China.
14. Smits, K. M., T. Sakaki, A. Limsuwat and T. H. Illangasekare (2009), Determination of the thermal properties of sands as affected by water content, drainage/wetting, and porosity conditions for sands with different grain sizes, 2009 Joint Assembly, The meeting of the Americas, May 24-27, Toronto, Ontario, Canada.
15. Smits, K. M., T. Sakaki, A. Limsuwat, and T. H. Illangasekare (2009), Determination of the thermal conductivity of sands under varying moisture, drainage/wetting, and porosity conditions- applications in near-surface soil moisture distribution analysis, Proceedings of the 29th Annual American Geophysical Union Hydrology Days, March 25-27, 2009, ed. J. A. Ramirez, pp. 58-66, Colorado State University, Fort Collins, CO.
16. Limsuwat, A., T. Sakaki, A. and T. H. Illangasekare (2009), Experimental quantification of bulk sampling volume of ECH2O soil moisture sensors, Proceedings of the 29th Annual American Geophysical Union Hydrology Days, March 25-27, 2009, ed. J. A. Ramirez, pp. 39-45, Colorado State University, Fort Collins, CO.
17. Frippiat, C. C., K. M. Smits, T. Sakaki, A. E. Holeyman, and T. H. Illangasekare (2009), Modeling the drainage of two- and three-dimensional heterogeneous media: influence of water mobility and air availability, European Geosciences Union (EGU) General Assembly 2009, Vienna, Austria, April 19-24.
18. Komatsu, M. and T. Sakaki (2009, Invited), Parameter estimation for numerical analysis of groundwater seepage and mass transport in porous media, International Symposium on Solution of Energy Problems from Environmental Point of View; Approach to Decreasing CO_2 Emission, January 16, Okayama University, Okayama, Japan.
19. Sakaki, T., A. Limsuwat, K. M. Smits, and T. H. Illangasekare (2008), Empirical two-point α-mixing model for calibrating dielectric soil moisture sensors in sandy materials, AGU Fall meeting, Poster No. H51H-0977, December 15-19, San Francisco, CA.
20. Frippiat, C. C., K. M. Smits, T. Sakaki, G. A. Zyvoloski, and T. H. Illangasekare (2008), Modeling spatial and temporal variability of

soil moisture in shallow depths of the vadose zone: A comparison of two and three dimensional simulations to capture relevant physical processes, AGU Fall meeting, Poster No. H13A-0885, December 15-19, San Francisco, CA., Outstanding Student Paper Award.
21. Illangasekare, T. H., T. Sakaki, K. M. Smits, and A. Limsuwat (2008, Invited), Soil Moisture Processes in the Near Surface Unsaturated Zone: Experimental Investigations in Multi-scale Test System, AGU Fall meeting, Poster No. H13FA-0984, December 15-19, San Francisco, CA.
22. Sakaki, T., C. C. Frippiat, T. H. Illangasekare, and M. Komatsu (2008), Geologic model construction in groundwater flow model calibration: A transitional probability approach for a non-stationary heterogeneous aquifer, Proceedings of the XXXVI IAH Congress 2008, p172-2:1-7, October 26-November 1, Toyama, Japan.
23. Sakaki, T., A. Limsuwat, C. C. Frippiat, and T. H. Illangasekare (2008), Near-surface water retention in the heterogeneous vadose zone subjected to evaporation, Proceedings of the XXXVI IAH Congress 2008, p172-1:1-6, October 26-November 1, Toyama, Japan. (PDF attached)
24. Frippiat, C. C., T. Sakaki, and T. H. Illangasekare (2008), Characterization of non-stationary heterogeneous hydraulic conductivity fields based on random and nested borehole data, Proceedings of the XXXVI IAH Congress 2008, p166:1-10, October 26-November 1, Toyama, Japan. (PDF attached)
25. Sakaki, T., G. Camps-Roach, D. M. O'Carroll, T.A. Newson and T.H. Illangasekare (2008), Direct quantification of dynamic effects in capillary pressure, Gordon Research Conference: Flow and Transport in Permeable Media, July 13-18, Oxford, United Kingdom.
26. Frippiat, C. C., T. Sakaki, and T. H. Illangasekare (2008), Experimental and numerical studies to evaluate the dependence of accuracy of subsurface model calibration on quality and quantity of observations, XVIIth International Conference on Computational Methods in Water Resources, July 6-10, San Francisco, California, (oral presentation only).
27. Smits, K. M., T. Sakaki, A. Limsuwat, C. C. Frippiat, and T. H. Illangasekare (2008), Spatial and temporal variability of water retention in shallow depths of vadose zone: Experimental investigation, Proceedings of the MODFLOW and More 2008, 188-192, May 19-21, Colorado School of Mines, Golden, CO. (PDF attached)
28. Limsuwat, A., T. Sakaki, and T. H. Illangasekare (2008), Water Retention Behavior in Heterogeneous Porous Media Under Water Table Fluctuations, Proceedings of the MODFLOW and More 2008, 193-197, May 19-21, Colorado School of Mines, Golden, CO. (PDF attached)
29. Sakaki, T., C. C. Frippiat, T. H. Illangasekare, and M. Komatsu (2008), Value of borehole data on geologic model construction for improving model calibration accuracy, Proceedings of the MODFLOW and More 2008, 439-443, May 19-21, Colorado School of Mines, Golden, CO.
30. Sakaki, T., D. M. O'Carroll, and T. H. Illangasekare (2007), Direct laboratory quantification of dynamic coefficient of a field soil for drainage and wetting cycles, AGU Fall meeting, Poster No. H53F-1486, December 10-14, San Francisco, CA.
31. Shlomi, S., T. Sakaki, T. H. Illangasekare, and A. Michalak (2007), Evaluation of geostatistical data assimilation methodologies for estimating groundwater plume distributions using 3D tracer tests, Proceedings of the 37th Mid-Atlantic Industrial & Hazardous Waste Conference, University of Cincinnati, Ohio, March 21-23, 2007; Sorial, G. A.; Bagtzoglou, A., Eds. University of Cincinnati, Ohio, 2007; pp 86-92.
32. Sakaki, T., A. Limsuwat, and T. H. Illangasekare (2007), Water retention behavior of sand as affected by a surrounding medium, The 27th Annual American Geophysical Union Hydrology Days, Poster No. 22, March 19-22, Colorado State University, Fort Collins, CO.
33. Illangasekare, T. H., T. Sakaki, and J. M. Terrés-Nicoli (2007), Intermediate-scale testing to study land-atmospheric interaction processes: Facility and experimental design, ARO Terrestrial Sciences Soil Moisture/Arid Lands Research Review Meeting, March 5-6, Fort Carson, CO.
34. Sakaki, T., and T. H. Illangasekare (2006), Retention curve measurement for sands using a TDR-based long column and modified Tempe cell, AGU Fall meeting, Poster No. H51-0462, December 11-15, San Francisco, CA.
35. Sakaki, T., M. Komatsu, and T. H. Illangasekare (2006), Preliminary exploration of dynamic effect in field soil retention curves: Direct laboratory quantification of material coefficient, AGU Fall meeting, Poster No. H51-0463, December 11-15, San Francisco, CA.
36. Sakaki, T., S. E. Howington, J. P. Hallberg, and T. H. Illangasekare (2006), Improved Subsurface Model Calibration Using Soft Data on Geologic Heterogeneity, AGU Fall meeting, Poster No. H43-0476, December 11-15, San Francisco, CA.
37. Sakaki, T., and T. H. Illangasekare (2006), Improved subsurface model calibration using soft data on geologic heterogeneity, Philadelphia Annual Meeting, October 22-25, Geological Society of America Abstracts with Programs, Vol. 38, No. 7, p. 111, Paper No. 40-9, Philadelphia Convention Center, Pennsylvania.
38. Sakaki, T., T. H. Illangasekare, and M. Komatsu (2006), Parameter estimation in a heterogeneous synthetic aquifer with different quantities of information on geologic features, Proceedings of the MODFLOW and More 2006, 71-75, May 22-24, Colorado School of Mines, Golden, CO.
39. Sakaki, T., and T. H. Illangasekare (2006), Tempe cell based static capillary pressure – saturation relationships for sands: Conventional averaging method vs. point measurement, The 26th Annual American Geophysical Union Hydrology Days, Poster No. 24, March 20-22, Colorado State University, Fort Collins, CO.
40. Sakaki, T., T. H. Illangasekare, and M. Komatsu (2005), Dependence of uncertainty in parameter estimation in non-stationary heterogeneous aquifers on the number and spatial distribution of observation wells, AGU Fall meeting, Poster No. H13D-1358, December 5-9, San Francisco, CA.

Number of Presentations: 40.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

(d) Manuscripts

Number of Manuscripts: 0.00

Patents Submitted

Patents Awarded

Awards

Illangasekare (2005-2010)

- Best Research Project Award 2005, SERDP/ESTCP (with B. Siegrist, M. Crimi and J. Marr)
- Elected to the Board of Trustees of the Consortium of Universities for Advancement of Hydrologic Sciences (CUAHSI), 2008.
- Elected by peers as the Vice-Chair of the Gordon Research Conference on Flow in Permeable Media to be held in 2010 and Chair to be held in 2012.
- Semi-finalist, National Security Science and Engineering Faculty Fellowship (NSSEFF), Department of Defense, 2010.
- Honorary Doctorate in Natural Science and Technology, Uppsala University, Sweden, 2010.

- Member of NAS/NRC Committee on " Future Options for Management in the Nation's Subsurface Remediation Effort"
- Member of NAS/NRC Committee on "Opportunities and Challenges for International Science at the USGS

- Recipient of Colorado School of Mines Senate Excellence in Research Award, August 2010.

. Editor, Water Resources Research

- Fellow, American Geophysical Union (AGU)
- Fellow, American Society of Civil Engineers (ASCE)
- Fellow, American Association for Advancement of Science (AAAS)

Graduate Students

NAME	PERCENT SUPPORTED
Toshi Sakaki	0.15
Kate Smits	0.50
FTE Equivalent:	**0.65**
Total Number:	**2**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Tissa Illangasekare	0.00	No
FTE Equivalent:	**0.00**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME	
Toshi Sakaki	
Total Number:	**1**

Names of personnel receiving PHDs

NAME	
Kathleen Smits	
Total Number:	**1**

Names of other research staff

NAME	PERCENT SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

1. Objectives and approach

This research is two-fold with the following focuses;
(1) Development of systematic approaches for calibration of subsurface transport models using hard and soft data on system characteristics and behavior (the original research focus, Tasks 1-5 below)
(2) Temporal and spatial distribution of soil moisture in the heterogeneous vadose zone as affected by near-surface atmospheric boundary conditions (additional work related to landmine detection, Tasks 6-8 below)

This first focus extends and combines recently-developed tools for parameter estimation and geostatistical simulation for use with groundwater flow and transport models used by the Army in field investigations involving groundwater quality and quantity. The second task focuses on improving our understanding and quantification of the distribution of soil moisture in the vadose zone as affected by land-atmospheric interaction, evaporation from soils, evapotranspiration and land mine detection. The primary aims of the project were to:

- Develop an improved understanding of how to add in a systematic way the geostatistical description of aquifer heterogeneity to the calibration process.
- Develop methods to condition parameter estimation to hard and soft data.
- Test our ability to use sparsely sampled data to determine calibration parameters at the large scale where simulations are conducted.
- Extend the findings/methods developed above for more complex problems involving multi-phase flow. More specifically, we will investigate spatial/temporal soil moisture behavior in the shallow subsurface (including around buried objects) under various conditions such as water table fluctuation/heat-induced evaporation etc. To accomplish this, a data set has to be generated under well-controlled conditions. Focusing on understanding and quantification of the distribution of soil moisture in the vadose zone (air-water two-phase flow problem), we added new tasks (Tasks 6, 7, and 8).
- The data sets generated in the highly complex system but under well-controlled conditions can also be used other modelers to test their inversion schemes.

Our approach uses existing forward and inverse modeling codes and new experimental data on head response to various pumping excitations and solute spills generated in a three-dimensional test bed facility at the Center for Experimental Study of Subsurface Environmental Processes (CESEP) at the Colorado School of Mines. The approach we use includes the following tasks, some of which have been revised/added:

Task 1: Forward modeling code selection

A number of computer codes that have the capability to simulate flow, reactive transport and mass transfer exist. The goal of this research task was to review existing models that were used by DOD and other government agencies for decision making and regulatory action.

Task 2: Review and evaluation of inverse codes

A primary tool that was used in this research was an inversion model that uses data on excitation and the corresponding responses to estimate the system parameters. The goal of this research task was to select the appropriate inversion code through initial testing with currently available data.

Task 3: Review of methods used in soft data collection and synthesis

In the original proposal this research task was proposed to gather information on the state or practice of model calibration at DOD sites. Discussions with WES collaborators, it was determined that the model calibration still relies on the use of both soft and hard data and inversion is not routinely used. Hence, the efforts under this task focused more on investigating the effect of quantity of hard and soft data on the parameter estimation accuracy (see Task 5).

Information such as degree to which formal inverse modeling approaches were used, steps in the calibration process, utilization of prior information, criteria used in determining good match, types of soft data used and degree of importance attached to such data, how issues of uncertainty were handled etc. will be gathered through a survey. In this work, data was categorized as either hard data or soft data, depending on the degree of quantitative uncertainty included in the data.

Hard Data: The data collected at a site on the past behavior or from controlled large-scale tests. The past behavior is recorded through observations of head or drawdown in wells and solute concentrations in monitoring wells. Controlled large-scale tests may include pumping tests and natural gradient tracer tests.

Soft Data: All other information that is either qualitative in nature or are collected at discrete points or localized areas in the system. The qualitative data includes, geology, large-scale stratigraphy and geophysical test results. Point data include data collected using soil cores and cone penetrometers. Localized data includes results from slug tests, push-pull tests and forced gradient tracer tests.

Task 4: Experimental design

A major component of this research project involved the design and use of experimental data generated in the laboratory to develop and validate calibration processes that systematically use both hard and soft data. The goal of this task was to generate a comprehensive data set under controlled conditions in intermediate scale test tanks. The key steps in the proposed method were:

- Pack a three-dimensional tank with a defined heterogeneity. Both structured and stochastically generated random packing configurations are used. Well-characterized test sands with accurately known hydraulic conductivities, dispersivity, porosity, reactive properties and retention characteristics are used.

- Flow and/or transport simulations are conducted to generate hard data on system response to various system excitations. These simulations correspond to water table drawdown due to pumping, plume generation due to a spill, dissolution from a NAPL spill, etc.

- Use the generated data to conduct automatic calibration using the appropriate simulator and inversion code. As the system characteristics are known exactly from the designed packing, it is possible to determine the accuracy of the model calibration and uncertainty of predictions.

- Soft data were introduced in a systematic manner to evaluate how the calibration got improved and uncertainty of predictions got reduced.

Task 5: Method and protocol development

This task involved the analysis of results from the previous tasks to develop a systematic procedure to calibrate models using both hard and soft data. The goal was to use the knowledge gained through analysis conducted using the experimental data to come out with a calibration protocol with validated guidelines. After reviewing the results from Tasks 1 through 4, it was inferred that the effect of quantity of hard and soft data on the parameter estimation accuracy had to be further investigated in detail, and we decided not to pursue the development of a general calibration protocol (based only on the data set that we have generated) that we originally proposed in the proposal. Therefore, in the new Task 5, we investigated value of soft and hard data for improving model calibration accuracy (e.g., Sakaki et al. [2008], PDF attached).

Task 6: A data set on soil moisture distribution in heterogeneous vadose zone

An understanding and quantification of the distribution of soil moisture in the vadose zone is important in many applications involving land-atmospheric interaction, evaporation from soils, evapotranspiration and land mine detection. Natural soil heterogeneity in combination with the flux conditions at the soil surface creates complex spatial and temporal distribution of soil moisture in the vadose zone. Capillary barrier effects at the interfaces of variation soil textures contribute to this complexity. We added the following tasks and generated data sets on soil moisture distribution; Task 6-1) in a simple two-dimensional heterogeneous system under drainage/wetting conditions (e.g., Limsuwat et al. [2008], PDF attached), Task 6-2) in simple two-dimensional heterogeneous systems subjected to evaporation at surface (e.g., Sakaki et al. [2008], PDF attached), and Task 6-3) in three-dimensional heterogeneous vadose zone (e.g., Smits et al. [2008], PDF attached). The goal of this research task was to develop a data set that describes the spatial and temporal distribution of soil moisture in simple heterogeneous systems and in three-dimension a spatially correlated random field under various boundary conditions (e.g, water table fluctuation, evaporation at the soil surface).

Task 7: Evaporation from 1D column: Experiment and modeling

The goal of this task was to perform controlled experiments under transient conditions of soil moisture and temperature using soil with accurately known hydraulic/thermal properties and use this data to test existing theories and develop appropriate numerical models. Water vapor flow under varying temperature gradients was implemented based on a concept that allows non-equilibrium liquid/gas phase change with gas phase vapor diffusion. In order to validate this new approach, we developed a long column apparatus equipped with a network of sensors and generated data under well-controlled thermal boundary conditions at the soil surface. Water saturation, capillary pressure, temperature, relative humidity and column weight to record total mass of water in the column were continuously monitored. Results from numerical simulations based on the conventional equilibrium and non-equilibrium approaches were compared with experimental data. This knowledge is applicable to many current environmental problems to include the simulation of contaminant transport and volatilization in the shallow subsurface and water content fluctuation in the vadose zone interacting with the atmosphere. For more details, see Smits et al.

Task 8: 2D tank experiment and modeling on moisture/temperature behavior around a buried object

The objectives of this work were; 1) to develop a unique large tank apparatus equipped with a network of recent sensor technologies for automated and continuous monitoring of moisture, temperature, and relative humidity, 2) to generate precision data under well-controlled transient heat boundary conditions to test a 2D heat and mass transfer model for soil containing a buried object over a diurnal cycle, 3) to compare model results and experimental data and 4) to expand our exploration of the effects of the soil environment on landmine detection by investigating the influence of the buried objects themselves, soil texture, and surface conditions on water content and soil temperatures above and below various objects buried at 10cm depth and away from it. A major finding of this study is that the thermal signature of a buried object strongly depends on the complex interaction between water content, soil thermal and hydraulic properties and geographical location. Temperature differences were, with some exceptions, larger in wet than in the dry sands, which suggests that soil water may help improve thermal signatures for some objects. Thermal and saturation contrasts were generally very different for a buried landmine than for other buried objects. It is our hope that this data and numerical model will improve the comprehension and interpretation of sensor imagery and lead to the development of more robust signal processing techniques. More details will be available in Smits et al. [manuscript to be submitted soon]

2. Transfer of data/knowledge

ARO-USACE Engineer Research and Development Center (ERDC) supported researchers at Colorado School of Mines (CSM) have provided the ERDC with experimental data sets on the 1) calibration of subsurface transport models using hard and soft data on system characteristics and behavior and 2) temporal and spatial distribution of soil moisture/temperature in the vadose zone that can be used to better understand fundamental processes and validate numerical models.

The PIs have been in contact with Dr. Stacy Howington and Jackie Hallberg at the WES to discuss how the data and research findings are to be used by the modeling group. A group that includes Dr. Stacy Howington and a research associate Ms. Jackie Hallberg visited the CESEP at CSM lab to discuss the data that have been collected and any additional sampling that might have to be done to meet their needs. We transferred the data we have generated to them. Ms. Hallberg is working on parameter estimation for WES's countermine work and for their other large simulators. In this research she has coupled their favorite flow/transport model (ADH) with PEST and is ready for a test. Dr. Howington also indicated Dr. Tim Kelley's interest in the dataset as a test of his optimization code. Dr. Howington has provided additional funding for this task.

The ERDC has been involved over the past 5 years in increasing landmine detection and reducing false alarms through the testing of automated target recognition software (ATRs) on synthetic IR imagery. This work has been funded through the Countermine, Near Surface Phenomenology, and GEOTACS programs. The work has focused on generating synthetic IR images which are added as test cases for ATR software. The production of synthetic imagery allows for a variety of scenarios to be tested that would be costly or difficult to test in the field. Because landmine sensors exploit soil and environmental conditions to discern between mines and other objects, most mine detection technologies require that the spatial and temporal variability of key environmental conditions such as climate, vegetation, soil type, depth of ground water table, and topography be understood. If these factors and the ability to model them in a variety of domains become well defined, then sensor and algorithm simulations can more realistically be tailored to particular operational scenarios and technologies. The experimental data sets provided by CSM provide a systematic experimental study of the effects of the near surface boundary conditions on soil moisture and temperature distributions in the shallow subsurface. Increasing our knowledge of the effects of geohydrologic/thermal properties and behaviors on the landmine signature will ultimately help to properly interpret sensor imagery. Experimental results can be used to validate numerical results from the ERDC's Computational TestBed.

Technology Transfer